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Influence of refractive index in particle sizing by light extinction spectrum

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Abstract

Light extinction spectrum (LES) is particularly preferred in particle sizing since it is a fast, nonintrusive, and easy-to-realize in situ measurement. The dispersion of particles is often neglected in LES based on particle sizing (LESPS). In this communication, we investigate the effect of the particle refractive index on the extinction properties of particles. We performed a quantitative analysis for the spectral extinction properties of particles with a known size distribution based on two different refractive indices (i.e., the refractive index at a certain wavelength and the dispersive model of refractive index). Our results show that, for water and glass droplets, the biggest difference of extinction values in the two cases is only 0.003 in the visible region; it has no significant influence in LESPS and can be neglected. For tear gas smoke particles, 2-chlorobenzalmalononitrile (CS), the biggest difference is 0.03 in the visible region, and it has great effect on the accuracy of LESPS. Therefore, taking the dispersion of particles into account, the measurement accuracy of particle size distribution and concentration can be improved.

Keywords: light extinction spectrum; extinction efficiency; tear gas smoke particles;

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1. Introduction

Light extinction spectrum is preferred used in particle sizing, because it is nondestructive and the results can be obtained rapidly. We can obtain more information of the particle sizing from the extinction spectra by LES. It can also make the results of the particle size distribution (PSD) (number frequency or volume frequency distribution) more accurate. The determination of extinction spectra [1,2] mainly depends on the extinction coefficient (Qext). The particles' Qext at different wavelengths is associated with the refractive index of that at different wavelengths. Then, in the current LES for the PSD, the refractive index of the particles is mainly considered as a constant. Based on the relationship between the particles' refractive index and light wavelength, in this paper we analyzed the influence of particles' (water, glass and CS droplets) dispersion characteristic to the extinction spectra. Experimental results of the LES for CS show that it has strong dispersion characteristic.

2. Principle of LSE

Assume that the incident light intensity is I_0 and the wavelength of light is λ. When the incident light traverses a particle system, its original intensity is reduced due to scatteration and absorption by the particles suspended in the medium [3]，it means that:

$$\ln(\mathrm{I}/\mathrm{I}_0) = -\frac{\pi}{4} l \int_a^b N(\mathrm{D})\,\mathrm{D}^2 Q_{ext}(\lambda, \mathrm{D}, \mathrm{m}(\lambda))\,\mathrm{dD} \tag{1}$$

Where I/I_0 is called extinction, in another word, extinction value, l is optical path length, a and b are the low limit and upper limit of the particle diameter range of PSD, N (D) is the number of the particles that size is D, Qext is the Extinction coefficient, which depends on the wavelength λ, the particle size D and the relative refractive index m(λ) of the particle to the disperse medium, and can be calculated by the Mie scattering theory for spherical particle [4]. The total volume of the particle can be calculated by:

$$V(\mathrm{D}) = \frac{\pi}{6} \int_a^b N(\mathrm{D})\,\mathrm{D}^3\,\mathrm{dD} \tag{2}$$

The number of the particles that size is D in LES can also be calculated by:

$$N(\mathrm{D}) = NN^*(\mathrm{D}, \bar{\mathrm{D}}, \mathrm{k}) \tag{3}$$

Which $N^*(D){=}N^*(D, \bar{D}, k)$ is characterized by the size parameter $\bar{D}$ and distribution parameter k . N is number of the particles. Substituting function (3) into function (1):

$$\ln(\mathrm{I}/\mathrm{I}_0) = -\frac{\pi}{4} lN \int_a^b N^*(\mathrm{D}, \bar{\mathrm{D}}, \mathrm{k})\,\mathrm{D}^2 Q_{ext}(\lambda, \mathrm{D}, \mathrm{m}(\lambda))\,\mathrm{dD} \tag{4}$$

The determination of Qext is a critical problem with LES. When we combine the dispersion relation of refractive index, the particles' Qext at different wavelengths is associated with the refractive index of that at different wavelengths.

3. The dispersion relation of refractive index

As two common materials, water and glass droplets' dispersion relation of refractive index have been discussed. The dispersion relation of pure water droplets under ambient temperature and atmosphere pressure is [6]:

$$m^2-1=\frac{0.5684027565\lambda^2}{\lambda^2-(0.005101829712)^2}+\frac{0.1726177391\lambda^2}{\lambda^2-(0.01821153936)^2}+\frac{0.02086189578\lambda^2}{\lambda^2-(0.02620722293)^2}+\frac{0.1130748688\lambda^2}{\lambda^2-(1.069792721)^2} \tag{5}$$

The dispersion relation of glass droplets (SiO2) is [7]:

$$m^2-1=\frac{0.6961663\lambda^2}{\lambda^2-(0.0684043)^2}+\frac{0.4079426\lambda^2}{\lambda^2-(0.1162414)^2}+\frac{0.8974784\lambda^2}{\lambda^2-(9.896161)^2} \tag{6}$$

As a result of our past work, the dispersion relation of CS is [8]:

$$m^2=2.1996-\frac{0.005}{\left(\lambda^2-4.489\times10^5\right)} \tag{7}$$

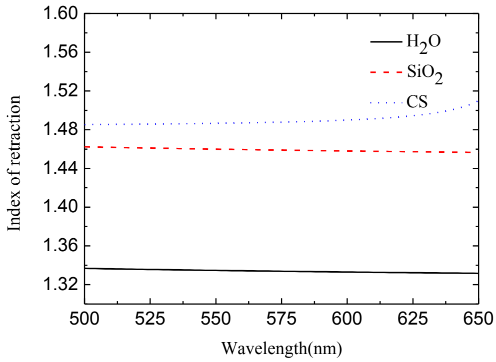

Fig. 1. Droplets' refractive index with the different wavelengths. The λ range is from 500nm to 650nm which is due to our work limit.

Table 1. Result of the droplets' refractive index curves varies with the different wavelength.

λ (nm)	H_2O	SiO_2	CS
500	1.3368	1.4623	1.4852
550	1.3347	1.4599	1.4866
600	1.333	1.458	1.4899
650	1.3317	1.4565	1.5099

From the Fig. 1 and Table 1, the refractive indexes of water droplets and glass droplets in the visible light range change small, the number of significant digits is the third. But for the CS in the visible light range, dispersion of the particles changes in effective digits in the second, which is big. If we don't take the dispersion considering, pick up the refractive index of a wavelength corresponding instead of the other band, e.g., m（λ=650nm）=1.510，So the maximum change of refractive index 8.7% when we calculate the particle distribution.

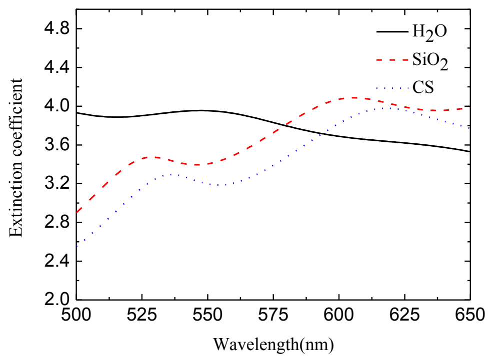

Fig. 2. Different particle extinction coefficient with the different wavelength (The particle size D=1000nm)

As indicated by Fig. 2, the water droplet Qext decreases monotonously with the wavelength increases overall, and glass droplets Qext shock with wavelength increase. The CS Qext varies with wavelength increasing volatility certain change, and the change is larger. So for the particles of different dispersion properties of materials, Qext in a certain spectral range is different with the change of wavelength.

4. Theoretical Calculations

The following is the analysis about the effect on the particle extinction characteristics under a certain particle size distribution, considering the dispersion or not. Import particle size distribution generation into the formula (4) and simulation respectively.

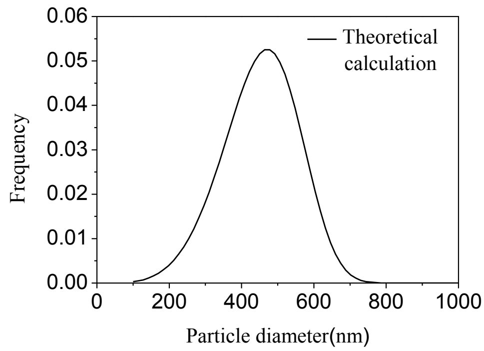

Fig. 3. Distribution of particle size by theoretical calculation (the size parameter $\bar{D}$=500nm， the distribution parameter k=5).

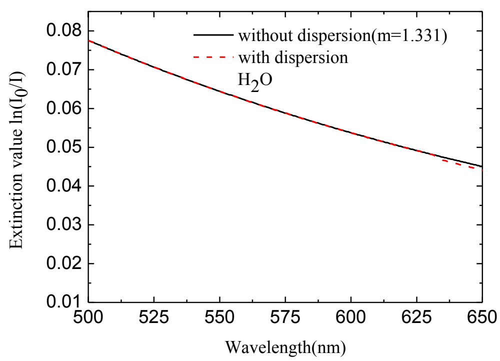

Fig. 4. Extinction spectrum of water droplets at the same particle size distribution one considered the dispersion, and the other one does not take into account.

From Fig.4 when λ<632nm, the lines in both cases do mostly overlap; when λ>632nm, the extinctions' difference is becoming bigger as the wavelength increases, when λ>632nm, the maximal difference is only 0.001.So the influence of the extinction spectrum by the water particles' dispersion can be ignore.

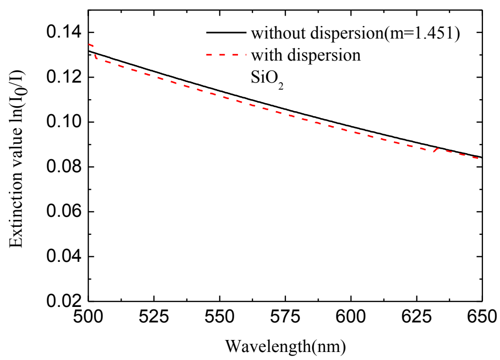

Fig. 5. Extinction spectrum of glass droplets at the same particle size distribution one considered the dispersion, and the other one does not take into account.

We can see in Fig.5 the extinction without dispersion is bigger than that with dispersion in the visible region. When λ=632nm, the minimum difference is 0.0004; when λ=500um, the maximal difference is 0.003. So the influence of the extinction spectrum by the glass droplets' dispersion can be ignored.

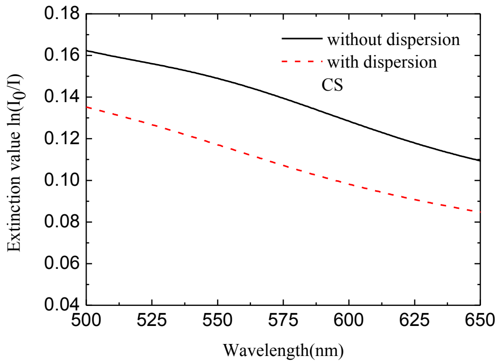

Fig. 6. Extinction spectrums of CS at the same particle size distribution one considered the dispersion, and the other one does not take into account.

Fig.6 plots that the lines in both cases do not overlap, the biggest gap is 0.03. So the influence of the extinction spectrum by the CS dispersion can't be ignored.

Above all, when we use LES to measure the particle size distribution of CS, we can't use a fixed refractive index values instead of refractive index values in the visible region. So we need to consider the effect of the particle dispersion to the extinction spectrum, and the effect of the results of LES.

5. Test methods and results

In this paper, we measured CS particle size distribution by Zhenzhong's experimental system [3]. Due to the inversion calculation software need to set up an important parameter that is the relative refractive index of the particles when it is running. At the beginning of passing into the CS (t=0), introduce the measured transmittance spectrum into the inversion software, based on the dispersion characteristics of CS, Analysis the difference between with and without dispersion on the calculation of particle size distribution. By calculating, the particle volume frequency distribution as shown in Fig. 7, the particle number frequency distribution as shown in Fig. 8.

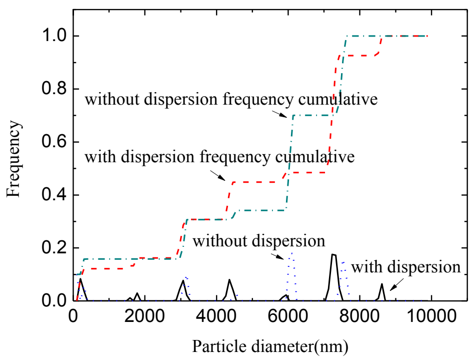

Fig. 7. Distribution of the V (D) when t=0.

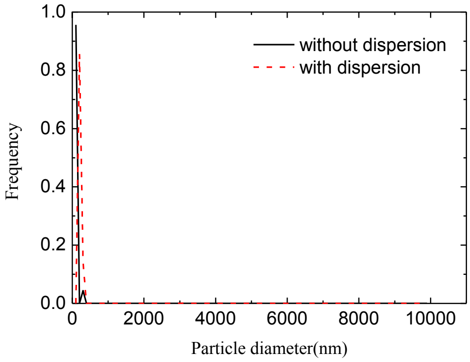

Fig. 8. Distribution of the N (D) when t=0.

The deviation of two cases'(consider the dispersion and doesn't consider the dispersion) particle size distribution results is large in Fig.7. When D =6μm, the biggest change caused by the cumulative frequency is 0.2, the maximum frequency change is 0.18. Therefore, for CS , if not consider particle dispersion characteristics, 8.7% of its refractive index changes can lead to 20% of the cumulative frequency, 18% of variation frequency. When we dealing with data use LES, we should consider the influence of dispersion characteristics of CS particle, Rather than use a fixed refractive index values instead of refractive index values within the whole band.

6. Conclusions

In this paper we learned that the influence of dispersion characteristics of water droplets and glass droplets is small when we calculate refractive index and Qext of the different materials. Based on CS dispersion curve, we know that the change of refractive index in the second effective digits, the particle dispersion is large. When we used to measure CS size distribution by LES, if we not consider particle dispersion characteristics, 8.7% of its refractive index changes can lead to 20% of the cumulative frequency, 18% of the variation frequency. As a result, it's very necessary to consider the dispersion characteristics of CS when we measure CS size distribution by LES.

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